



MOLECULAR FOUNDRY USER MEETING

AUGUST 11–12, 2016



Thursday, August 11

Plenary Session

8:00 am	Registration/Breakfast	B50 Auditorium
9:00 am	Welcome - User Executive Committee	Building 50 Auditorium
9:05 am	Molecular Foundry Update <i>Jeffrey Neaton, Director of the Molecular Foundry, Berkeley Lab; Professor of Physics, UC Berkeley</i>	
9:30 am	Keynote Address: Evolving Click Chemistry → SuFEx <i>K. Barry Sharpless, W. M. Keck Professor of Chemistry, The Scripps Research Institute</i>	
10:10 am	Nanoparticle-Polymer Conjugates for Near-Infrared Biomolecular Detection <i>Markita Landry, UC Berkeley</i>	
10:30 am	Refreshment Break	Tent
11:00 am	New Capabilities at the Molecular Foundry <i>Mike Brady, Emory Chan, Shaul Aloni, Frank Ogletree, Peter Ercius, Alex Muller, Frances Allen, David Prendergast</i>	Building 50 Auditorium
11:40 am	Core-Shell Micro-Tube Array for Closing the Artificial Photosynthesis Cycle on a Nanometer Scale <i>Eran Edri, Berkeley Lab</i>	
12:00 pm	Fabricating and Actuating DNA Origami Mechanisms <i>Alexander Marras, The Ohio State University</i>	
12:20 pm	Staff Award — User Executive Committee	
12:30 pm	Lunch	Tent
1:30 pm	Town Hall Meeting (users only)	Building 70A, Room 3377
2:00 pm	Keynote Address: New Insights into Oxygen Electrochemical Reactions on (La,Sr)MnO₃ <i>Sossina M. Haile, Walter P. Murphy Professor of Materials Science and Engineering, Professor of Applied Physics, Northwestern University</i>	Building 50 Auditorium
2:40 pm	Study of Plasmonic Behavior of Nanoantennas via Transmission Electron Microscopy <i>Braulio Archanjo, National Institute of Metrology, Quality and Technology (Brazil)</i>	
3:00 pm	New Half-Metallic Ferromagnets Induced by a Quantum Critical Point from First Principles <i>Sinead Griffin, Berkeley Lab and UC Berkeley</i>	
3:20 pm	Probing Atomic and Electronic Structure Effects of Halide Composition in Perovskite Photovoltaics <i>Walter Drisdell, Berkeley Lab</i>	
3:40 pm	The Joint Genome Institute & Emerging Single-Cell Genomic Technologies <i>Devin Doud, Berkeley Lab</i>	
4:00 pm	Poster Session & Exhibitor Fair Refreshments Served	Building 54 Patio/Cafeteria
6:30 pm	End of Poster Session	



MOLECULAR FOUNDRY USER MEETING

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Friday, August 12

Symposia

8:00 AM	Late Registration/Breakfast	B50 Auditorium
9:00 AM	Morning Symposia Commence: 9:00 AM – 12:30 PM: Biological and Soft Material Assemblies 9:00 AM – 12:30 PM: Making, Measuring and Manipulating Two-Dimensional Matter 9:00 AM – 12:30 PM: Structural and Functional Diversity in Porous Soft Materials 9:00 AM – 12:30 PM: Tackling Challenges of Imaging Materials Functionality: Symposium on Current Imaging Technology	Various (See Symposia detail sheet)
10:30 AM	Refreshment Break	Tent
11:00 AM	Morning Symposia Continue	Various
12:30 PM	Lunch	Tent
1:30 PM	Afternoon Symposia Commence: 1:30 PM – 5:00 PM: Energy Storage Materials: Synthesis, Characterization and Modeling 1:30 PM – 5:00 PM: Playing with Photons at the Nanoscale 1:30 PM – 5:00 PM: Product-Driven Research at the Molecular Foundry 1:30 PM – 5:00 PM: Tackling Challenges of Imaging Materials Functionality: Workshop on Future and Current Needs at the MF	Various (See Symposia detail sheet)
3:00 PM	Refreshment Break	Tent
3:30 PM	Afternoon Symposia Continue	Various
5:00 PM	Meeting Adjourned	

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Friday, August 12

Morning Symposia

Biological and Soft Material Assemblies

Location: **Building 54, Room 130 (Perseverance Hall)**

Organizer: Ron Zuckermann, Caroline Ajo-Franklin, Bruce Cohen

Biopolymers and synthetic polymers can assemble into an incredible diversity of hierarchical nano architectures that can perform a host of sophisticated functions. But control over their design, synthesis and characterization still presents a major challenge. Many Foundry users are addressing key aspects of this problem. In this symposium we will discuss strategies to improve soft material computational design tools, synthesis and supra-molecular assembly mechanisms, and their characterization by microscopy and scattering techniques.

9:00 AM	Discovery of Affinity Reagents from Combinatorial Libraries of Functionalized Peptoid Nanosheets <i>Mark Kline, Berkeley Lab</i>
9:30 AM	Computational Design of Self-Assembling Protein Nanomaterials <i>Jorge Fallas, University of Washington</i>
10:00 AM	Biological Recognition of f-element Complexes: From Spectroscopic Probes to Therapeutics <i>Rebecca Abergel, Berkeley Lab</i>
10:30 AM	Refreshment Break
11:00 AM	Nanoscale Insights Into Microscale Combat; Mechanisms of Interbacterial Warfare <i>Joseph Mougous, University of Washington</i>
11:30 AM	Self-Assembling Protein Nanosheets for Selective Metal Recovery <i>Marimikel Charrier, Berkeley Lab</i>
12:00 PM	Accessing New Supramolecular Assemblies Through de Novo Peptide Designs <i>Ryan Spencer, UC Irvine</i>

Making, Measuring and Manipulating Two-Dimensional Matter

Location: **Building 70A, Room 3377**

Organizers: Adam Schwartzberg, Nathan Hohman

Abstracting single monolayers from two-dimensional (2D) van der Waals solids like graphene and the transition metal dichalcogenides has created new classes of metallic and semiconducting materials that have attracted broad interest for new applications enabled by their unique properties. Of note, high carrier mobilities and strong spatial screening dependence between charge carriers in 1D and 2D systems and unusually large optical cross sections have attracted interest for applications ranging from photovoltaics to valleytronics. This multidisciplinary symposium will explore the rapidly evolving science of making new and old 2D materials, measuring their properties, and manipulating them into complex heterostructures in pursuit of new applications for these cutting-edge materials.

9:00 AM	Two-Dimensional Crystal Growth and Polymorphism in Metal Sulfides <i>Zafer Mutlu, UC Riverside</i>
9:30 AM	A Novel Approach for Fabricating Nano Devices Based on Transition Metal Dichalcogenides <i>Christoph Kastl, Berkeley Lab</i>
10:00 AM	Molecular Transport in Membranes Made by Stacking 2D Graphene Oxide Nanosheets <i>Baoxia Mi, UC Berkeley</i>
10:30 AM	Refreshment Break
11:00 AM	2D Crystals for Smart Life <i>Kaustav Banerjee, UC Santa Barbara</i>
11:55 AM	Graphene Membranes for Atmospheric Pressure Photoelectron Spectroscopy <i>Robert Weatherup, Berkeley Lab</i>

Structural and Functional Diversity in Porous Soft Materials

Location: **Building 2, Room 100B**

Organizers: Yi Liu, David Prendergast

Recent advances in the field of porous soft materials represent one of the most rapidly growing research areas worldwide, which demonstrate great potential in achieving structural and functional diversity. Great strides have been made in the design, synthesis, simulation and characterization of representative porous soft material classes and their hybrids, such as metal-organic frameworks, covalent organic frameworks, supramolecular organic frameworks, polymers with intrinsic microporosity, etc. The structural diversity has led to promising energy applications, including gas adsorption and separation, CO₂ and water splitting, optoelectronics and photovoltaics, and energy storage, to name a few. This symposium will bring together broad expertise from chemists, material scientists and physicists to foster collaborations and forge new opportunities that will advance the related research fields.

9:00 AM	Electrochemical CO ₂ Reduction Over Precisely Fabricated Metal Organic Frameworks and Covalent Organic Frameworks <i>Yingbo Zhao, UC Berkeley</i>
9:30 AM	Investigating Nanostructured Organic Frameworks and Porous Polymers with X-ray Scattering <i>Michael Brady, Berkeley Lab</i>
10:00 AM	The Importance of a Precise Crystal Structure for Simulating Gas Adsorption in Nanoporous Materials <i>Keith Lawler, University of Nevada, Las Vegas</i>
10:30 AM	Refreshment Break
11:00 AM	Electrohydrodynamic-Assisted Assembly of Hierarchically Structured, 3D Graphene Monoliths for Efficient Energy Harvesting and Solar Conversions <i>Vincent Tung, UC Merced</i>
11:30 AM	The Computation-Ready Experimental Metal-Organic Framework Database: Development and Applications <i>Jeffrey Camp, Georgia Institute of Technology</i>
12:00 PM	Metal-Organic Frameworks to Enable Low-Cost Distributed Chemical Sensors <i>David Britt, Matrix Sensors</i>

Tackling Challenges of Imaging Materials Functionality: Symposium on Current Imaging Technology

Location: **Building 50 Auditorium**

Organizers: Peter Ercius, Francesca Toma, Alex Weber-Bargioni

Co-localization of the morphological, chemical, and functional information through advanced nanoscale characterization represents one of the most significant challenges in materials characterization. The Molecular Foundry includes advanced measurement equipment and in-house expertise taking great strides in this direction. In an effort to pair up problems and solutions, this symposium will present cutting edge research equipment and techniques in imaging techniques available at the Molecular Foundry. Researchers involved in nanoscale synthesis and theory are encouraged to attend in an effort to identify potential underutilized, unidentified or currently unavailable techniques for their specific scientific applications. The afternoon workshop discussion will be geared towards aligning MF efforts to answering these questions.

9:00 AM	Cathodoluminescence at the Movies: Revealing Nanoscale Dynamics in Solid and Liquid Solutions <i>Naomi Ginsberg, Berkeley Lab and UC Berkeley</i>
9:30 AM	Facet-Dependent Photovoltaic Efficiency Variations in Perovskite Grains <i>Sibel Leblebici, Berkeley Lab</i>
10:00 AM	First Principles Modeling of Structural and Electronic Properties of Hybrid Halide Perovskites <i>Linn Leppert, Berkeley Lab</i>
10:30 AM	Refreshment Break
11:00 AM	Spatial Mapping of 2D Valence Bands at the MAESTRO Beamline at ALS <i>Eli Rotenberg, Berkeley Lab</i>
11:30 AM	Probing Properties of Matter at the Nanoscale by Scanning Electron Nanodiffraction <i>Roberto dos Reis, Berkeley Lab</i>
12:00 PM	Imaging of Biomolecules and Bioinspired Materials at the Molecular Foundry <i>Paul Ashby, Berkeley Lab</i>



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Friday, August 12

Afternoon Symposia

Energy Storage Materials: Synthesis, Characterization and Modeling

Location: **Building 70A, Room 3377**

Organizer: Alpesh Shukla

Advances in electrification of vehicles and successful implementation of an electricity grid that efficiently utilizes renewable energy sources is largely dependent on the development of materials that would result in energy storage systems with substantially superior energy density, cycle life and safety compared to those provided by the state-of-the-art batteries. This symposium will focus on the materials aspects of the components of batteries such as cathode, electrode and electrolyte and interactions between them. This symposium will include topics related to the energy storage materials that include, but are not limited to synthesis of novel materials, phase transformations in electrode materials, study of interfaces and materials discovery. These studies would showcase several capabilities of Molecular Foundry such as synthesis of nanomaterials, multi-scale microscopy and spectroscopy techniques and materials modeling.

1:30 PM	Composite of Two-Dimensional Titanium Carbonitride “MXene” and Nano-Sulfur as Cathode for Li-S Batteries <i>Michael Naguib, Oak Ridge National Laboratory</i>
2:00 PM	Crystal-Based Microscopy and Spectroscopy Diagnostics for Lithium-Ion Battery Cathode Development <i>Guoying Chen, Berkeley Lab</i>
2:30 PM	Electronic Structure, Entropic and Quantum Effects in Nanoscale Aqueous Systems <i>Tod Pascal, Lawrence Berkeley National Laboratory</i>
2:45 PM	Effect of Non-Uniform Porosity on Lithium Plating <i>Sun Ung Kim, Robert Bosch Research and Technology Center</i>
3:00 PM	Refreshment Break
3:30 PM	NMC Cathode and LLZO Electrolyte Studies <i>Marca Doeff, Berkeley Lab</i>
4:15 PM	TiS ₂ /CNT Hybrid Supercapacitors-Battery Breaks the Limit of Supercapacitors Based on Aqueous Electrolyte <i>Xining Zang, UC Berkeley</i>
4:30 PM	Discussion: Future of Energy Storage Research

Playing with Photons at the Nanoscale

Location: **Building 54, Room 130 (Perseverance Hall)**

Organizers: Stefano Cabrini, Jim Schuck

The field of nanophotonics uses the plasmonic response of metals, as well as the precise organization of high refractive index structures, to shape and focus light far below the diffraction limit. The ability to fabricate, test, simulate, and understand nanophotonic devices and structures has attracted a broad user community asking fundamental questions about plasmonic antenna shape, new materials and their influence on photonic responses and new geometries. New applications are now possible and many more are very close to be achievable.

1:30 PM	Hot Electron and Surface Plasmon Drive Chemical Reactions <i>Jeong Y. Park, Korea Advanced Institute of Science and Technology</i>
2:05 PM	Campanile-Inspired 3D Near Field Optical Probes <i>Alexander Koshelev, aBeam Technologies</i>
2:40 PM	Probing Sub-5 nm Gap Plasmon Using Collapsible Nano-Fingers <i>Boxiang Song, University of Southern California</i>
3:00 PM	Refreshment Break
3:30 PM	Systematic Design in Hybrid Chalcogenides <i>J. Nathan Hohman, Berkeley Lab</i>
4:00 PM	Shape Approaches for Enhancing Plasmon Propagation in Grapheme <i>Roman Krahne, Italian Institute of Technology</i>
4:20 PM	Energy-Looping Nanoparticles: Harnessing Excited State Absorption for Deep-tissue Imaging <i>Emory Chan, Berkeley Lab</i>
4:40 PM	TiN for Improved Plasmonics with Plasma-Enhanced Atomic Layer Deposition <i>Lauren Otto, University of Minnesota</i>

Product-Driven Research at the Molecular Foundry

Location: **Building 2, Room 100B**

Organizers: **Kristen Aramthanapon, Brett A. Helms**

The Molecular Foundry supports a broad user base with industry ties. Our early stage start-up users have made strategic use of Foundry resources to accelerate their discovery efforts and to advance those discoveries into products that further seed their business' growth. Larger businesses likewise see value in engaging the Foundry, where locally grown expertise and world-leading instrumentation can bring new insight into the fundamental scientific aspects of complex materials and industrial processes. This symposium seeks to highlight first-hand how our users from industry are gaining the perspective they need to be successful while at the Foundry. This might include a discussion of how to balance needs to both do leading-edge science while also meeting the business' milestones on schedule and how industry and its objectives help to advance new areas of science not typically considered in an academic setting.

1:30 PM	High-Throughput Materials Discovery for Advanced Additive Manufacturing Raymond Weitekamp, polySpectra
1:50 PM	Incorporating Metal-Organic Frameworks into Electromechanical Devices for Consumer Products David Britt, Matrix Sensors
2:10 PM	Towards Efficient, Scalable Electricity Generation Using Thermionic Energy Conversion Jared Schwede, Spark Thermionics
2:30 PM	Anti-Fouling, Self-Cleaning Coatings for Heat Exchangers Sebnem Inceoglu Yilmaz, Nano Hydrophobics
2:50 PM	Development of Metal-Organic Frameworks for Applications in Industrial Gas Separations Thomas McDonald, Mosaic Materials
3:10 PM	Refreshment Break
3:30 PM	Bio-Based Monomers for Bulk Polymer Applications Deepak Dugar, Visolis
3:50 PM	Exosome-Tunneling Nanotube Constructs for Cellular Rescue in Neurodegenerative Diseases Greg Maguire, BioRegenerative Sciences
4:10 PM	Functionalizable Fluorescent Nanodiamonds for Bioimaging Joyce Wahba, Bikanta
4:30 PM	From the Arctic Ocean to Industry: X-Therma's Biomimetic Anti-Ice Nanomaterial Xiaoxi Wei, X-Therma

Tackling Challenges of Imaging Materials Functionality: Workshop on Future and Current Needs at the Molecular Foundry

Location: **Building 50 Auditorium**

Organizers: **Peter Ercius, Francesca Toma, Alex Weber-Bargioni**

Discussion will focus on current and future needs including in situ and in operando techniques to image functionality with active participation of all attendees to identify scientific questions that the MF could potentially tackle. What are properties or functionalities scientists would like to probe or map but are not available today? What are approaches that are currently feasible or could be feasible with collaborative projects combining collective efforts that the MF excels in.

1:30 PM	The Future of TEM is Faster, with Clearly More Data to Analyze Andy Minor, Berkeley Lab and UC Berkeley
2:00 PM	Advanced Low Energy Electron Microscopy to Image Functional Materials Andreas Schmid, Berkeley Lab
2:30 PM	Quasi-Operando Imaging of the Surface Structure-Product Selectivity Functionality of Electrocatalysts by Seriatim ECSTM-DEMS Manuel Soriaga, California Institute of Technology
3:00 PM	Refreshment Break
3:30 PM	Three Dimensional Localization of Nanoscale Battery Reactions Using Soft X-ray Tomography David Shapiro, Berkeley Lab
4:00 PM	Development of Theoretical Models to Correlate Theory and Observables David Prendergast, Berkeley Lab
4:30 PM	Through a Flask, Darkly: Imaging Needs From a Chemical Perspective Jeff Urban, Berkeley Lab